Theory of inelastic scattering from magnetic impurities

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We use the numerical renormalization group method to calculate the single particle matrix elements $\mathcal{T}$ of the many body T-matrix of the conduction electrons scattered by a magnetic impurity at $T = 0$ temperature. Since $\mathcal{T}$ determines both the total and the elastic, spin-diagonal scattering cross sections, we are able to compute the full energy-, spin- and magnetic field dependence of the inelastic scattering cross section, $\sigma_{\mathrm{inel}}(\omega)$. We find an almost linear frequency dependence of $\sigma_{\mathrm{inel}}(\omega)$ below the Kondo temperature, T_K, which crosses over to a $\sim \omega^2$ behavior only at extremely low energies. Our method can be generalized to other quantum impurity models.

Quantum mechanical phase coherence in mesoscopic structures is destroyed due to inelastic processes, where excitations such as spin waves, electron-hole excitations, phonons, *etc.*, are created in the environment with a certain probability, thus leading to dephasing and loss of quantum coherence after a time $\sim \tau_\varphi$ [1]. In some weak localization measurements of the dephasing time τ_φ down to very low temperatures, a surprising saturation of τ_φ has been observed [2]. This unexpected saturation remained a puzzle for a long time until recently, when further experiments on mesoscopic quantum wires confirmed that the most likely candidates to produce this surprising behavior are magnetic impurities [3, 4]. These magnetic impurities seem to be present even in samples of extreme purity, and unavoidably lead to inelastic scattering and the dephasing of charge carriers.

Theoretical calculations also confirmed these expectations and showed that the experimental data can be quantitatively explained assuming weak inelastic scattering off Kondo impurities [5, 6]. These calculations, though, were performed in the weak coupling regime, *i.e.*, at energies higher than the Kondo temperature, T_K. However, Nozières Fermi liquid theory teaches us that well below T_K the magnetic impurity spin is screened by the conduction electrons, and there it acts simply as a strong but conventional potential scatterer, and thus produces no inelastic scattering. Therefore the inelastic scattering rate from magnetic impurities is expected to show a *peak* around T_K and then drop to zero well below T_K [7].

These observations motivate us to study the complete energy dependence of the inelastic scattering rate off a magnetic impurity. Here we shall focus on the simplest possible case of $T = 0$ temperature, where the inelastic scattering rate can be defined as follows: Assume that we have a single scattering impurity at the origin and we create an incoming flux of electrons with momentum $\mathbf{k}$, spin σ, and energy E above the Fermi energy, far away from the origin. This incoming flux can be scattered off the impurity in two different ways: (*i*) Either the electrons scatter *elastically* (both energy and spin unchanged) with

a scattering cross section $\sigma_{\mathrm{el}}(E)$ into an outgoing single particle state, without perturbing the environment, or (*ii*) they scatter off *inelastically* with a corresponding cross section $\sigma_{\mathrm{inel}}(E)$, *i.e.*, and they leave behind some electron-hole or spin excitations.

In the present paper, we show how the full energy and magnetic field dependence of $\sigma_{\mathrm{inel}}(E)$ can be determined. The basic idea is simple: The single particle matrix elements of the many-body T-matrix, $\langle \mathbf{k} \, \sigma | \hat{T} | \mathbf{k}' \, \sigma' \rangle$, determine the elastic cross section, but they are also related to the total scattering cross section, $\sigma_{\mathrm{tot}} = \sigma_{\mathrm{el}} + \sigma_{\mathrm{inel}}$ through the optical theorem. Therefore, we only have to find a way to compute the $\langle \mathbf{k} \, \sigma | \hat{T} | \mathbf{k}' \, \sigma' \rangle$'s to obtain the inelastic scattering cross section as the difference of the total and elastic scattering cross sections:

$$\sigma_{\mathrm{inel}}^\sigma = \sigma_{\mathrm{total}}^\sigma - \sigma_{\mathrm{el}}^\sigma \,. \tag{1}$$

To determine $\langle \mathbf{k} \, \sigma | \hat{T} | \mathbf{k}' \, \sigma' \rangle$, we shall first relate them through the reduction formulas to some local correlation functions [8], which we shall then calculate using the non-perturbative method of the numerical renormalization group (NRG) [9]. Though here we shall focus exclusively on the case of $T = 0$ temperature, where excitations are created from the vacuum state [10], our discussions carry over, with some modifications, to the case of finite temperatures too [11].

To be specific, we first consider the Anderson model, but our method is rather general and applies to practically any local quantum impurity problem. We write the Hamiltonian as $H = H_0 + H_{\mathrm{int}}$, where H_0 denotes the 'free' quadratic part of the Hamiltonian,

$$H_0 = \sum_\sigma \epsilon_d d_\sigma^\dagger d_\sigma + \sum_{\sigma,\mathbf{k}} \xi(\mathbf{k}) c_{\mathbf{k}\,\sigma}^\dagger c_{\mathbf{k}\,\sigma} \,,$$

and H_{int} stands for the on-site Hubbard interaction and hybridization

$$H_{\mathrm{int}} = U \, n_\uparrow n_\downarrow + V \sum_{\sigma,\mathbf{k}} \left(c_{\mathbf{k}\,\sigma}^\dagger d_\sigma + \mathrm{h.c.} \right) \,, \tag{2}$$

with $n_\sigma = d_\sigma^\dagger d_\sigma$. The operator $c_{\mathbf{k}\,\sigma}^\dagger$ creates an electron in a plane wave state with momentum $\mathbf{k}$, energy $\xi(\mathbf{k}) =$

$\frac{\mathbf{k}^2}{2m} - \mu$ and spin σ, while d_σ is the annihilation operator of the d-electron.

We proceed to define incoming and outgoing *scattering states* as well as the corresponding field operators and Hilbert spaces [8]. As the impurity is local, the interaction switches off far away and the 'in' and 'out' states are eigenstates of the full Hamiltonian with the asymptotic boundary condition of behaving as plane waves in the $x \to -\infty$ and $x \to \infty$ limits, respectively. The many-body S-matrix and the T-matrix elements are then simply defined in terms of the overlaps of the incoming and outgoing scattering states,

$$\langle b, \text{out}|a, \text{in}\rangle \equiv \langle b, \text{in}|\hat{S}|a, \text{in}\rangle \ , \qquad (3)$$

$$\hat{S} = 1 + i\,\hat{T} \ . \qquad (4)$$

In the interaction representation, the explicit form of the S-matrix is given by the well-known expression $\hat{S} = \text{T}\exp\{-i\int_{-\infty}^{\infty} H_{\text{int}}(t)\,dt\}$, where T is the time ordering operator.

Since we are primarily interested in the single-particle matrix elements of $\hat{T}$, we consider the case where asymptotically $|a, \text{in}\rangle$ is simply a single particle low energy excitation of the free vacuum defined by $H(x = -\infty) \to H_0$, having momentum $\mathbf{k}$ and spin σ: $|a, \text{in}\rangle = |\mathbf{k}, \sigma\rangle$. Then the single-particle matrix elements of the T-matrix read

$$\langle \mathbf{k}, \sigma|\hat{T}|\mathbf{k}', \sigma'\rangle = 2\pi\delta(\xi(\mathbf{k}) - \xi(\mathbf{k}'))\langle \mathbf{k}, \sigma|\mathcal{T}|\mathbf{k}', \sigma'\rangle \ , \quad (5)$$

where we separated a Dirac delta contribution due to energy conservation and defined the on-shell T-matrix $\mathcal{T}$. Next, following the manipulations of Ref. 8 we re-express the off-diagonal ($\mathbf{k} \neq \mathbf{k}'$) matrix elements of the T-matrix as:

$$\langle \mathbf{k}\,\sigma|\mathcal{T}|\mathbf{k}'\sigma'\rangle = \qquad\qquad\qquad (6)$$
$$-s\,G_0^{-1}(\xi, s\,\mathbf{k})\,G_{s\sigma,s\sigma'}(\xi, s\,\mathbf{k}, s\,\mathbf{k}')\,G_0^{-1}(\xi, s\,\mathbf{k}') \ ,$$

where $s = \text{sgn}\,\xi$ distinguishes electron-like excitations from hole-like excitations, $G_0^{-1} = i\frac{\partial}{\partial t} + \mu + \frac{1}{2m}\nabla^2$ denotes the inverse of the free Green's function, and G is the time-ordered single particle Green's function. The meaning of Eq. (6) becomes more transparent in the diagrammatic language of Fig. 1: As indicated by the large, thin crosses there, one has to drop the contributions of the two external legs of all scattering diagrams to the single electron Green's function and the rest is just the on-shell single particle matrix element of the many-body T-matrix. In the particular case of the Anderson model, $\mathcal{T}$ does not depend on the direction of incoming and outgoing momenta, and a simple Dyson equation relates it to the d-level's time-ordered propagator (see Fig. 1)

$$\mathcal{T}^\sigma(\omega) = -s\,V^2\,G_d^{s\cdot\sigma}(\omega) \ , \qquad (7)$$

where $s = \text{sgn}\,\omega$ and we allowed for spin-dependence due to the presence of an external magnetic field B. Eq. (7)
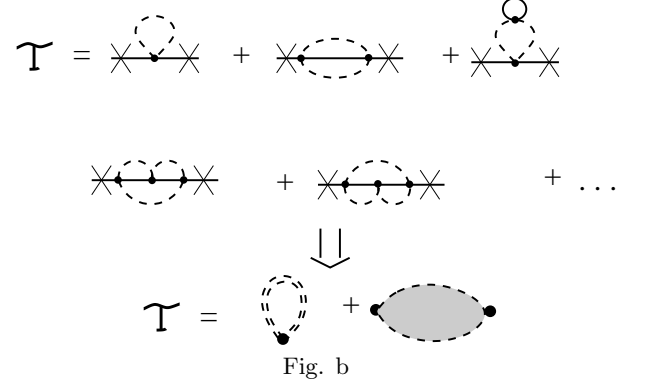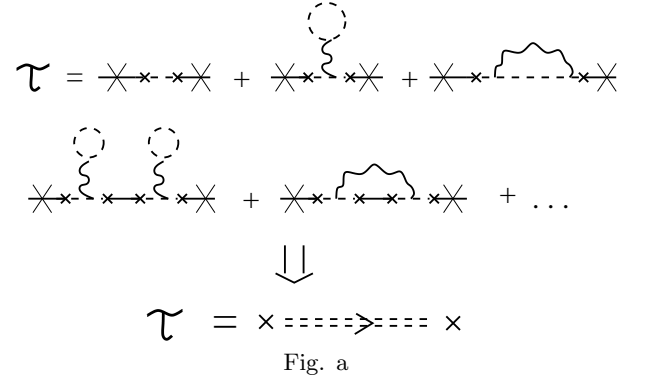

Fig. a

Fig. b

FIG. 1: (a) Diagrammatic derivation of Eq. (7). Dashed and continuous lines denote the bare propagators of the d-level and the conduction electrons, small fat crosses stand for hybridization V, and wavy lines denote the on-site interaction U. (b) Diagrammatic representation of the T-matrix in the Kondo problem. Dashed lines denote pseudofermion propagators and describe the evolution of the impurity spin, while continuous lines denote free conduction electron propagators. Filled circles stand for the exchange interaction J. The first term of the T-matrix is simply proportional to the expectation value of the impurity spin, it is frequency independent, and vanishes in the absence of magnetic field. The second term can be identified as the composite fermions correlation function.

has also been derived in a somewhat different way in Ref. 17.

According to the optical theorem, the spin-dependent total scattering cross section is given by the imaginary part of the diagonal matrix elements of the $\mathcal{T}$-matrix:

$$\sigma_{\text{total}}^\sigma = \frac{2}{v_F}\text{Im}\langle \mathbf{p}\sigma|\mathcal{T}|\mathbf{p}\sigma\rangle \ , \qquad (8)$$

where v_F denotes the Fermi velocity. The elastic scattering cross section, on the other hand, is related to the square of $\mathcal{T}$:

$$\sigma_{\text{el}}^\sigma = \frac{1}{v_F}\int \frac{d\mathbf{p}'}{(2\pi)^3}2\pi\,\delta(\xi' - \xi)|\langle \mathbf{p}'\sigma|\mathcal{T}|\mathbf{p}\sigma\rangle|^2 \ . \quad (9)$$

Once these two cross-sections are known, we can compute the inelastic cross section σ_{inel} through Eq. (1).

It is instructive to rewrite σ_{inel} in case of the Anderson model. For electrons we have

$$\sigma_{\text{inel}}^{\sigma}(\omega > 0) = \frac{4\pi}{k_F^2} \left[-\frac{\Gamma}{2} \text{Im} \, G_d^{\sigma} - \left(\frac{\Gamma}{2}\right)^2 |G_d^{\sigma}|^2 \right], \quad (10)$$

where $\Gamma = 2\pi V^2 \varrho_0$ denotes the width of the d-level and $\varrho_0 = k_F^2/2\pi^2 v_F$ is the conduction electrons' density of states for one spin direction. For $B = 0$, this expression reduces to

$$\sigma_{\text{inel}}(\omega > 0) = \frac{2\pi}{k_F^2} \frac{\Gamma \, (-\Sigma''(\omega))}{(\omega - \epsilon_d - \Sigma'(\omega))^2 + (\Sigma''(\omega) - \frac{\Gamma}{2})^2} ,$$

where Σ' and Σ'' denote the real and imaginary parts of the d-propagator's self-energy. The analytical properties of the Green's function imply that the above expression is always positive and it only vanishes where Σ'' becomes zero. Furthermore, the Fermi liquid theory of Yamada and Yoshida tells us that $\Sigma'' \sim \omega^2$ as $\omega \to 0$, and thus the inelastic scattering rate vanishes as ω^2 at the Fermi energy. Note that at the same time the total scattering cross section approaches the unitary limit.

To compute the full behavior of σ_{inel} we determined the $\mathcal{T}$-matrix using the numerical renormalization group method [9]. Since we were dominantly interested in the low-energy universal regime of the Anderson model, we took the $U/2 = -\epsilon_d \to \infty$ limit and performed the calculations using the Kondo Hamiltonian,

$$H_K = \frac{J}{2} \sum_{\mathbf{k}, \mathbf{k}'} \vec{S} \cdot (c_{\mathbf{k}\sigma}^{\dagger} \vec{\sigma}_{\sigma\sigma'} c_{\mathbf{k}'\sigma'}^{\dagger}) . \quad (11)$$

Up to an overall normalization factor, the low-energy part of the spectral function of the original d-level propagator in the Anderson model can be shown to correspond to the spectral function of the following composite fermion operator in the Kondo model [12], $F_{\sigma} \equiv \sum_{\sigma', \mathbf{k}} \vec{S} \cdot \vec{\sigma}_{\sigma\sigma'} c_{\mathbf{k}\sigma'}$. (For a diagrammatic proof, see Fig. 1). The imaginary part of $G_d \sim \mathcal{T}$ can thus be determined by simply computing the spectral function $\varrho_F(\omega)$ of the composite fermion numerically, and then a Hilbert transform can be used to get the real part of G_d and thus the full $\mathcal{T}$-matrix. In all these calculations it is essential to have high quality data. It is also crucial to determine the normalization factor of ΓG_d correctly. This can be done by using the Fermi liquid relation, $-\text{Im} \, \Gamma G_d^{\sigma}(\omega = 0^+) = 2 \sin^2 \delta_{\sigma}$, with δ_{σ} the phase shift at the Fermi energy. We extracted the latter directly from the finite size NRG spectrum of the Kondo model [9, 13].

Our results for the case of no external magnetic field are shown in Fig. 2. Most of the scattering is inelastic at energies above the Kondo energy, $|\omega| > T_K$. Decreasing the energy of the incoming electrons (holes), the total scattering cross section increases and, at energies below the Kondo scale, it finally saturates at a value $\sigma_0 = 4\pi/k_F^2$. This behavior must be contrasted
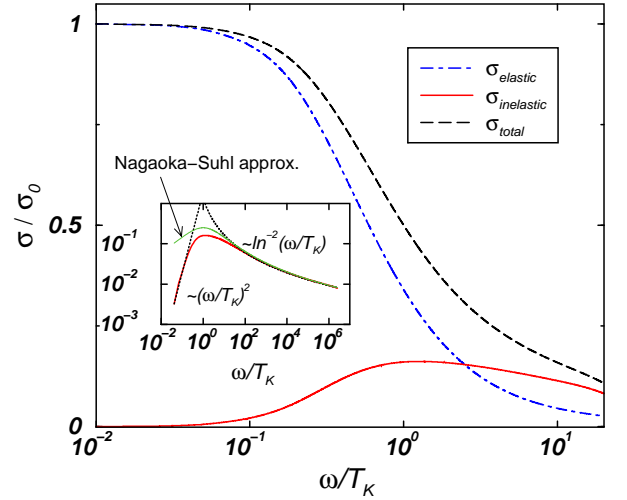

FIG. 2: Inelastic, elastic, and total scattering cross sections in units of $\sigma_0 = 4\pi/k_F^2$ at $T = 0$ and in the absence of magnetic field, as a function of the logarithm of the energy of the incoming electron. Only the electronic contribution ($\omega > 0$) is plotted. σ_{inel} only has a very weak (logarithmic) energy dependence above T_K, scales approximately linearly with ω for $0.01 \, T_K < \omega < T_K$, and scales as $\sim \omega^2$ for $\omega < 0.01 \, T_K$. The inset shows the $\sim \omega^2$ and $\sigma_{\text{inel}} \sim 1/\ln^2(T_K/\omega)$ regimes for $\omega \ll T_K$ and $\omega \gg T_K$, respectively.

to the inelastic scattering rate, which slowly increases as ω decreases, has a broad maximum around T_K then suddenly drops and vanishes at the Fermi energy. On linear energy scales (see Fig. 3), σ_{inel} varies rather slowly above T_K, is very large even at $\omega \sim 20 T_K$, and vanishes rather suddenly around $\omega \sim T_K$. For very small energies $\sigma_{\text{inel}} \sim \omega^2$, in agreement with Fermi liquid theory, however, this quadratic behavior appears only at very low energies, and σ_{inel} is almost linear for $0.1 \, T_K < \omega < T_K$. At energies $\omega \gg T_K$ the inelastic rate is simply dominated by energy-conserving spin-flip scattering, and is therefore expected to scale as $\sim 1/\ln^2(T_K/\omega)$, as we indeed find numerically. Note that the Nagaoka-Suhl approximation [15] is only appropriate for $\omega \gg T_K$ (see inset of Fig. 2).

We also computed the inelastic scattering rate in the presence of a local magnetic field, B, directed downwards along the z-axis (see Fig. 3). In this case there is a dramatic difference between the inelastic scattering properties of spin up and spin down particles. Already a small field, $B \sim 0.1 T_K$ results in a strong spin-dependence of the inelastic scattering, but for $B \sim T_K$, this difference is even more dramatic. At this field the spin of the magnetic impurity is practically aligned with the external field and points downwards. Therefore an incoming spin down particle (electron or hole) is unable to flip the impurity spin. More precisely, only higher order inelastic processes can result in a flip of the local impurity spin.
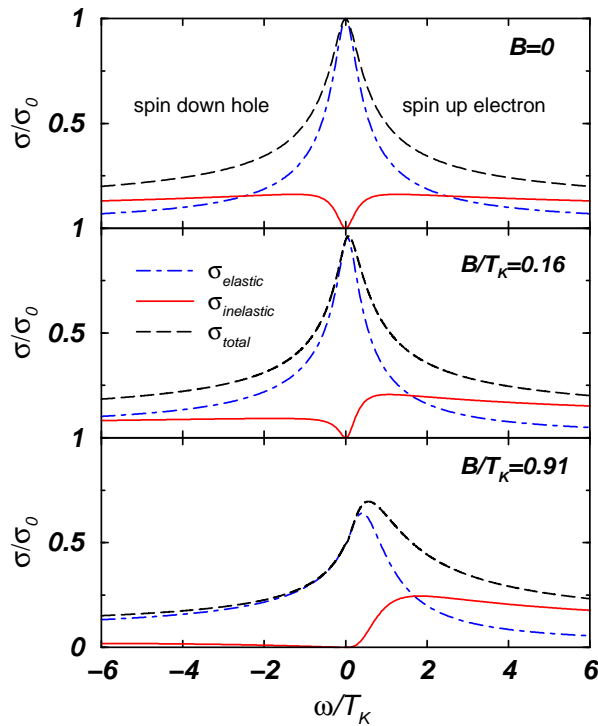
FIG. 3: Energy dependence of spin-dependent elastic and inelastic scattering rates in units of $\sigma_0 = 4\pi/k_F^2$, at $T = 0$ and in the presence of a local magnetic field B.

This is, however, not true for spin up particles: An incoming spin up electron can exchange its spin with the magnetic impurity in a first order process, resulting in a maximum in the inelastic scattering cross section around $\omega \sim B$ for spin up electrons and holes and a very broad inelastic background for $\omega > B$.

Though here we mostly focused on the simplest cases of the Anderson and the single channel spin $S = 1/2$ Kondo models at $T = 0$ temperature, our formalism can be extended to other models and to finite temperatures as well [11]. In particular, while for some quantum impurity models no simple diagrammatic theory is available, the composite fermion's spectral function can be computed in any Kondo-type model to obtain the matrix elements of the T-matrix, and the renormalization group flow of the eigenvalues of the S-matrix can be studied in all these cases [11]. While usually a thorough numerical analysis is needed to understand the full behavior of σ_{inel}, in some models simple analytical results can also be obtained. In the specific case of the 2-channel Kondo problem, *e.g.*, we know that the single particle matrix elements of the S-matrix identically vanish at the Fermi energy, $\omega = 0$ [14, 16]. This implies that $\varrho_0 \mathcal{T}^{2\text{CK}}(\omega = 0) = i/\pi$ and leads to the rather surprising relation at the Fermi level, $\sigma_{\text{inel}}^{2\text{CK}} = \sigma_{\text{el}}^{2\text{CK}} = \sigma_{\text{tot}}^{2\text{CK}}/2$: Though the S-matrix vanishes identically, half of the scattering processes remain elastic.

The non-vanishing inelastic scattering rate is characteristic of non-Fermi liquid quantum impurity models. Application of any finite magnetic field drives the 2-channel Kondo model to a Fermi liquid fixed point, and gives rise to a vanishing inelastic scattering rate at the Fermi energy.

We have to emphasize that, though they must be related, the inelastic scattering rate we computed is *not* identical to the dephasing rate measured in weak localization experiments [2], since the former incorporates spin-flip scattering processes as well as the creation of electron-hole pairs. While we only computed $\sigma_{\text{inel}}(\omega, T = 0)$, we expect that $\sigma_{\text{inel}}(\omega = 0, T)$ has a very similar form. In this sense, our finding that the inelastic scattering rate is roughly linear with ω for $0.05\, T_K < \omega < 0.5 T_K$ agrees qualitatively with the recent experimental results of Ref. 18.

In summary, we have shown how the full energy and magnetic field behavior of the $T = 0$ inelastic scattering rate can be computed by exploiting the reduction formulas and then using the powerful machinery of numerical renormalization group to compute the single particle matrix elements of the many-body T-matrix. We have shown that the Fermi liquid theory of Yamada and Yoshida directly implies a quadratically vanishing inelastic scattering rate at the Fermi energy in the specific case of the Anderson model. Scattering properties of the Kondo model have been computed by calculating the composite Fermion's spectral function. Our numerical calculations show that the abovementioned $\sigma_{\text{inel}} \sim \omega^2$ regime appears only at energies well below the Kondo temperature. In a magnetic field $B > T_K$ the inelastic scattering is very sensitive to the spin of the scattered single-particle excitation.

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